Supporting Information

Solid-state nanocasting synthesis of ordered mesoporous CoN_x-carbon catalysts for highly efficient hydrogenation of nitro compounds

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Experimental Procedures

Chemicals: Nitrobenzene (≥ 99.0 %), cobalt nitrate hexahydrate (≥ 98.5 %), sucrose, sodium hydroxide (96.0 %), and ethyl silicate (≥ 28.4 % SiO_2) were obtained from Sinopharm Chemical Reagent Co., Ltd. Histidine, 2-nitrobenzaldehyde and the tri-block copolymer P123 were purchased from Sigma Aldrich. Ethyl acetate (~ 99.5 %) was provided by Aladdin. Methanol absolute was obtained from Enox. 4-nitroacetophenone (~ 98%), 4-chloronitrobenzene (~ 98%), 4-nitrostyrene (~ 97%) were purchased from Energy Chemical. 4-iodonitrobenzene (~ 98%) was purchased from Macklin Biochemical Co., Ltd. 4-tert-butyl-1-nitrobenzene (> 97%) was obtained from Tokyo Chemical Industry Co., Ltd. Nitrocyclohexane (~ 97%) was purchased from Beijing Bellingway Technology Co., Ltd.

Supporting figures and tables

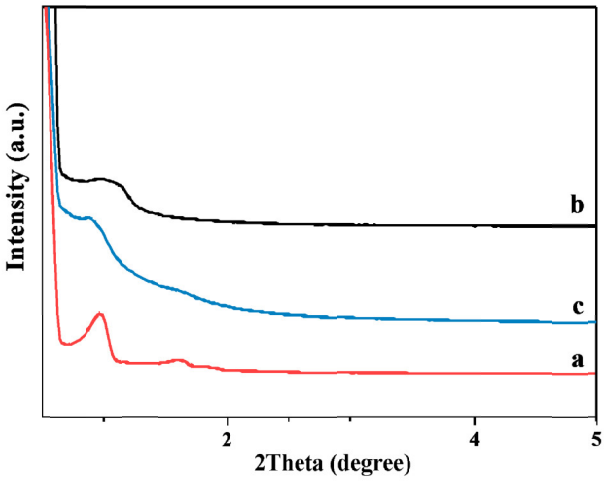

Figure S1. Small-angle XRD patterns of the ordered mesoporous silica SBA-15 template (a), the representative catalyst CoN_x-OMC-800 (b), and the control sample Co-OMC-800 (c), respectively.

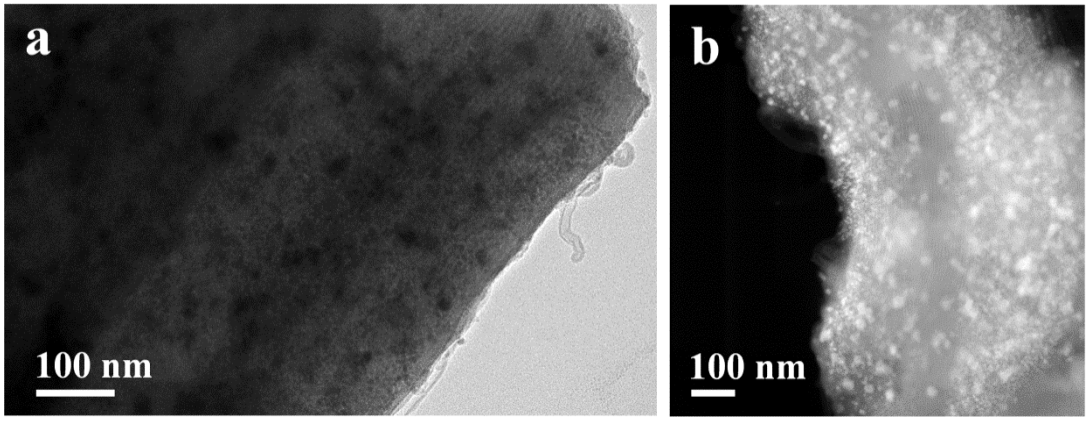

Figure S2. TEM (a) and STEM (b) images of the carbonized CoN_x-OMC-800@SBA-15 composite before the HF treatment.

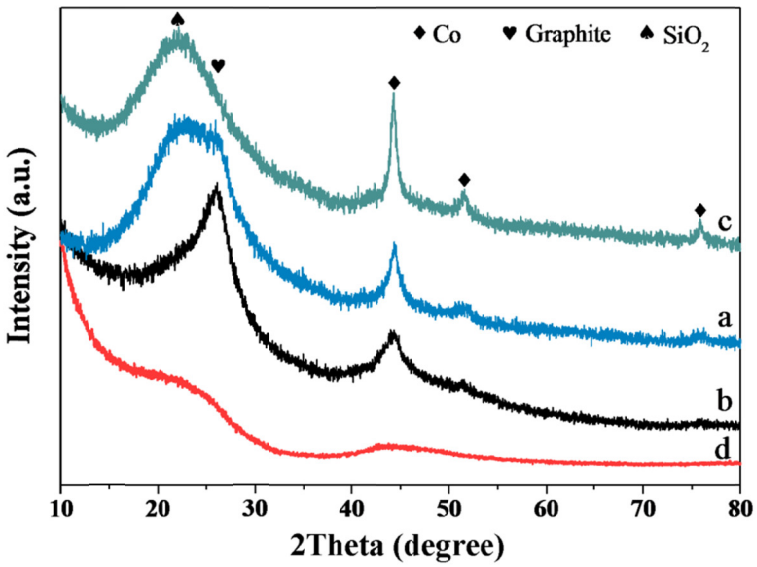

Figure S3. Wide-angle XRD patterns of the representative catalyst CoN_x-OMC-800 (b) and the control sample Co-OMC-800 (d), and their corresponding carbonized composites before the HF acid treatment (a, c), respectively.

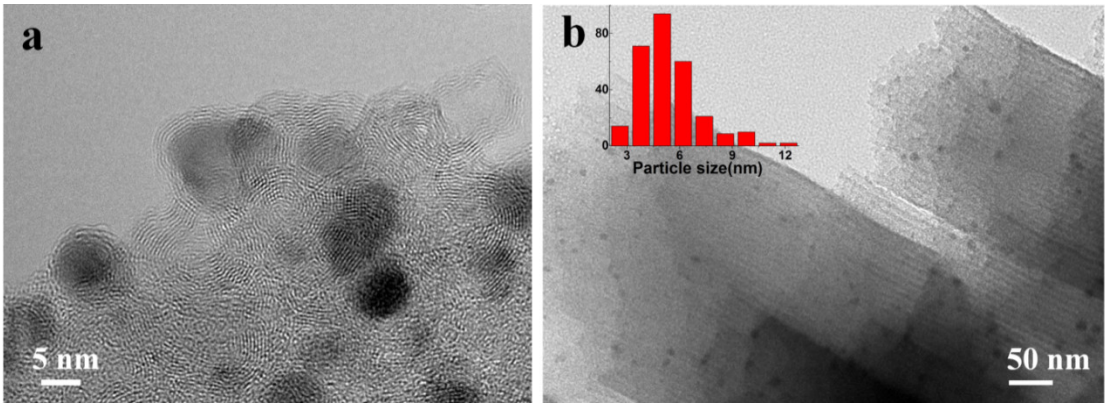

Figure S4. HRTEM (a) and TEM (b) images of the representative catalyst CoN_x-OMC-800. Inset (b) is the nanoparticle size distribution histogram.

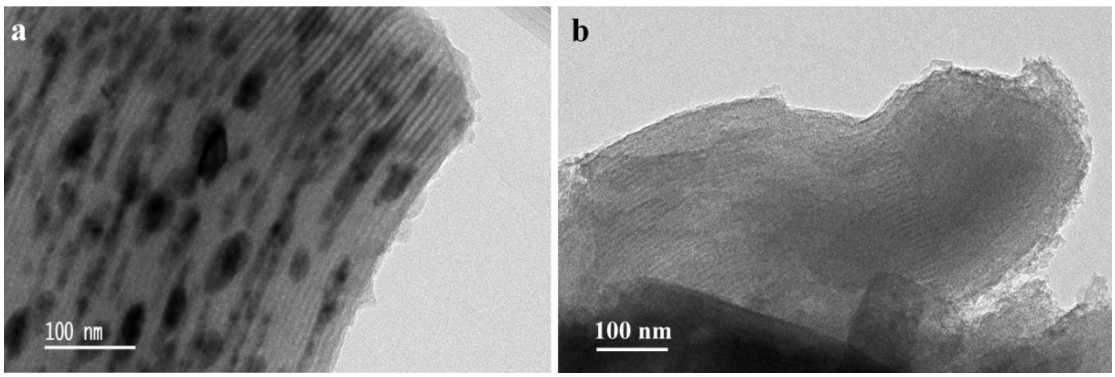

Figure S5. TEM images of the control sample Co-OMC-800 before (a) and (b) after the HF acid treatment.

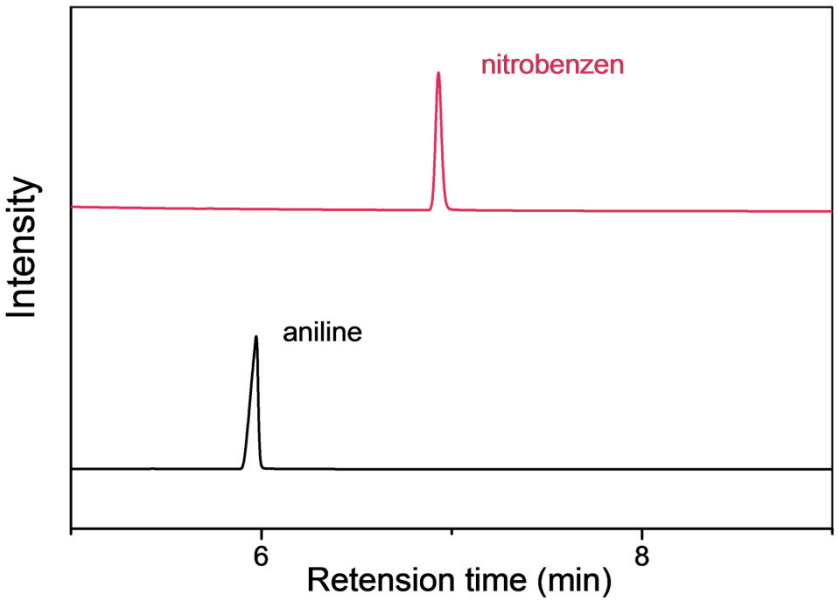

Figure S6. GC spectra of the nitrobenzenethe starting nitrobenzene solution (top curve) and the product (bottom curve) after the hydrogenation of nitrobenzene over the CoN_x-OMC-800 catalyst.

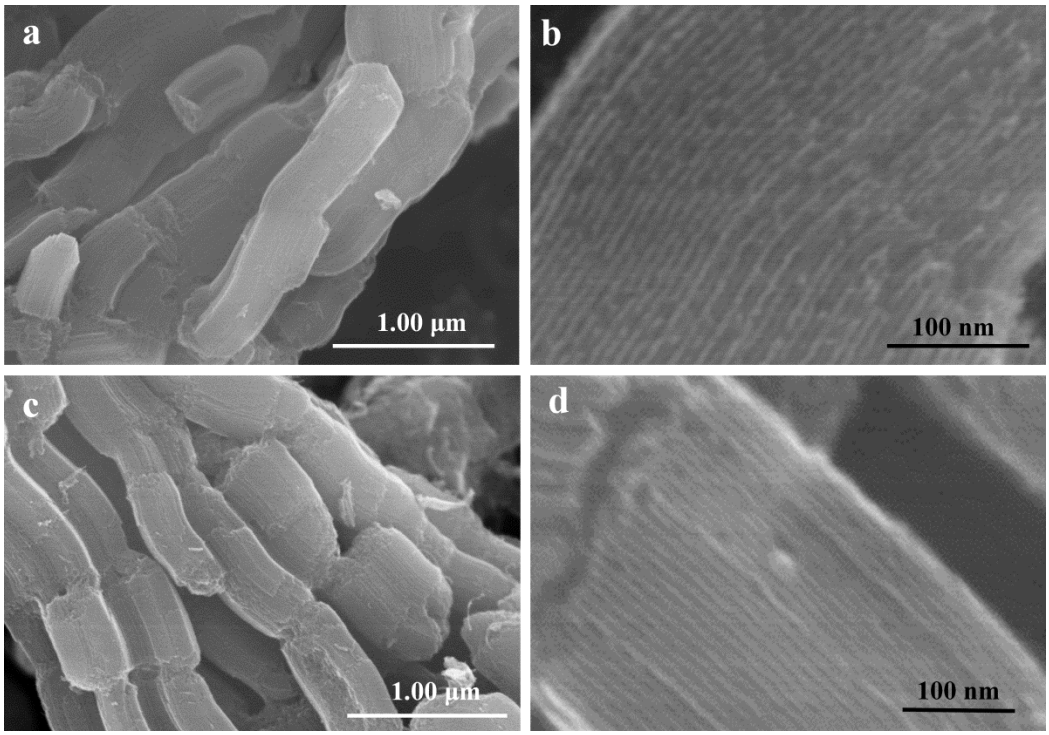

Figure S7. SEM (a, c) and HRSEM (b, d) images of the samples CoN_x-OMC-700 (a, b) and CoN_x-OMC-900 (c, d), respectively.

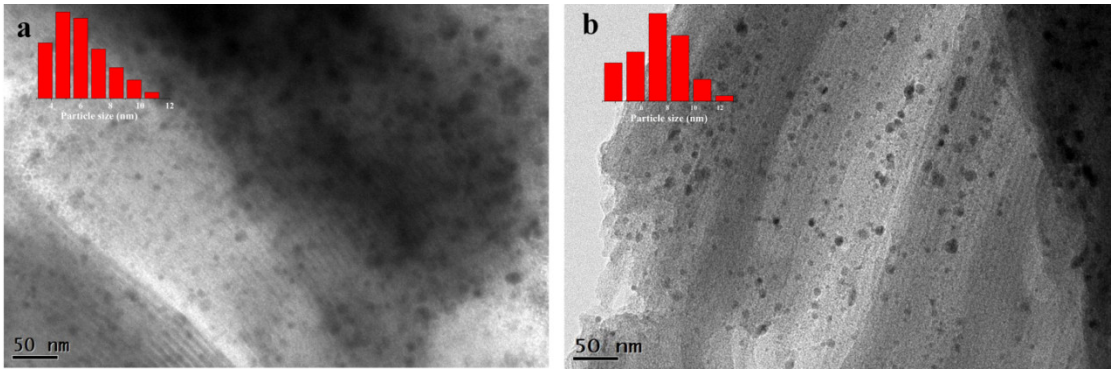

Figure S8. TEM images of the samples CoN_x-OMC-700 (a) and CoN_x-OMC-900 (b). Insets (a, b) are the corresponding nanoparticle size distribution histogram.

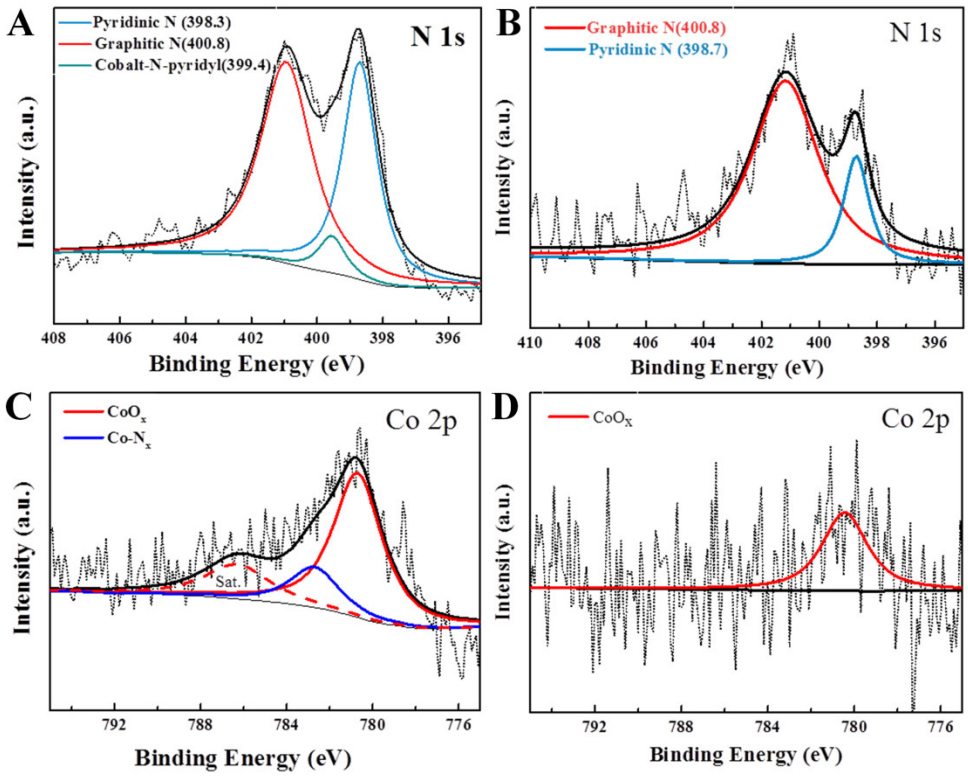

Figure S9. N 1s (A, B) and Co 2p (C, D) XPS spectra of the samples CoN_x-OMC-700 (A, C) and CoN_x-OMC-900 (B, D), respectively.

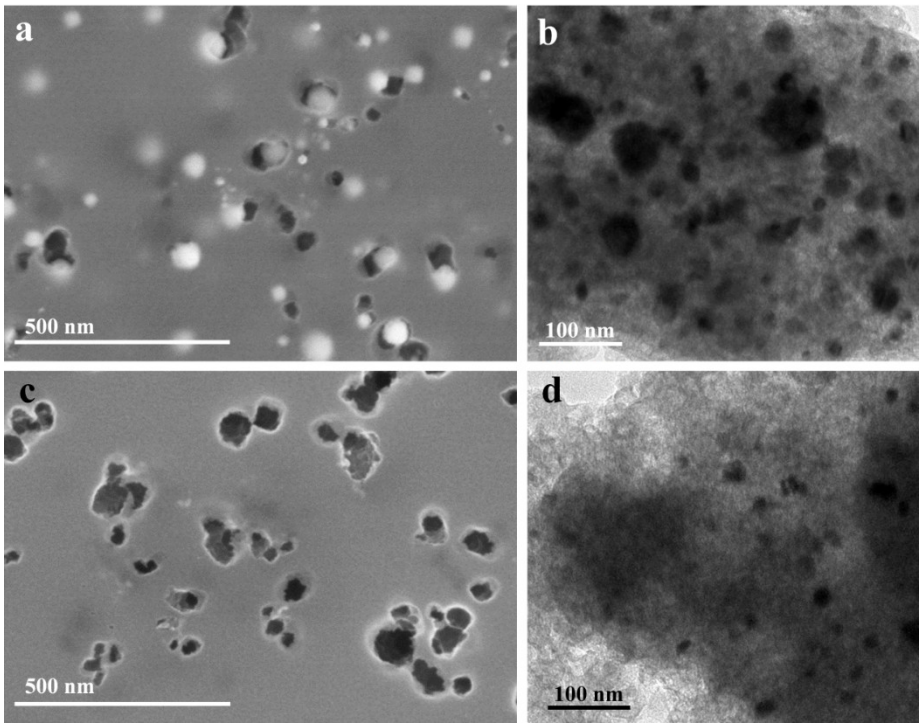

Figure S10. SEM (a, c) and TEM (b, d) images of the control sample CoN_x-C-800 before (a, b) and after (c, d) the HF acid treatment.

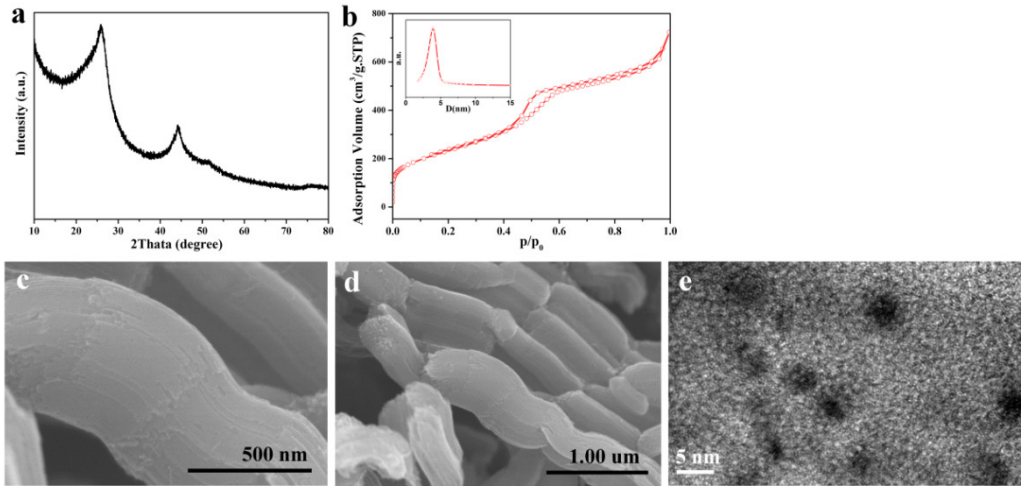

Figure S11. Wide-angle XRD pattern (a), N_2 sorption isotherms (b), SEM (c, d) and HRTEM (d) images of the representative catalyst CoN_x-OMC-800 after 7 runs of catalytic reaction.

Table S1. Comparison of the catalytic performance between the representative catalyst CoN_x-OMC-800 and typical reported catalysts in literature toward the hydrogenation of nitrobenzene with molecular H_2 as the hydrogen source.

Catalyst	Temperature (°C)	Reaction time (h)	H_2 pressure (bar)	Conversion (%)	Solvent	Ref
CoN_x-OMC-800	110	1.5	5	100	H_2O	This work
CoN_x-OMC-800 *	110	1.5	5	100	H_2O	This work
Co–N_x/C-800-AT	110	1.5	3.5	100	H_2O	1
Co-L1/C	110	12	50	> 99	THF	2
Co-SiCN	110	15	50	> 99	THF	3
Co-colloid	80	4	25	89.8	THF	4
Co@mesoNC	110	2	30	> 99	ethanol	5
CoOx@NCNTs	110	2.5	30	> 99	ethanol	6
Zr12-TPDC-CoH	110	42	40	100	toluene	7
0.08%Pt/FeOx-R200 *	40	1	3	100	toluene	8
Pd@Beta *	110	0.75	10	100	toluene	10
PdsNC/PN-CeO_2 *	80	2	5	> 99.9	methanol	11

* Substrate = 4-nitrochlorobenzene

Supporting references

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